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A microstructure-guided numerical approach to evaluate strain sensing and damage detection ability of random heterogeneous self-sensing structural materials

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1. Introduction

Structural Health monitoring (SHM) provides valuable information on the reliability and safety of the structures and it can help develop strategies to save the structures before critical damage threatens the structural integrity [\[1,2\]](#page--1-0). Strain- and damage-sensing are integral aspects of SHM. Most of the load-bearing structures are very sensitive to damage and it can cause catastrophic failures leading to immense loss of life and property $[1,3]$. Therefore costly routine inspections have been used for maintenance of these structures. Traditionally, various non-destructive testing (NDT) techniques such as ultrasound testing, radiographic tests (X-ray) etc. have been used, although they are impractical and expensive for large structures. Thus, there has been a need for a real-time mixed global/local damage-sensing approach. For realscale industrial structures, use of smart composites is gaining popularity in recent times for strain-sensing in structures [\[4–6\]](#page--1-1). In particular, such smart composites achieve damage-sensing capability by utilizing piezoresistivity which is an electromechanical phenomenon that enables certain electrically conductive composites to respond electrically under

the influence of strain $[7-14]$. Electrical resistance methods in these composites have been shown to be sensitive to minor and microscopic changes that include defects or damage [\[10,14–16\].](#page--1-3)

Design of such smart materials requires a reliable numerical method that can predict electro-mechanical response at different length scales. This paper presents a comprehensive microstructure-guided electromechanical response prediction framework for a large class of smart heterogeneous materials using finite element modelling. In particular, the numerical framework is applied towards prediction of strain-sensing efficiencies in smart cementitious composites for infrastructure applications. In cement-based materials self-sensing capability has been achieved using carbon fibers, steel fibers and carbon nanotubes [\[7,9,14,17\].](#page--1-2) Although a variety of experimental studies $[8-15,18]$ report on electro-mechanical response of these systems under tension and compression, limited studies exist on prediction of strain-sensing and damage-detection efficiency in such self-sensing cementitious materials which is the primary goal of this research paper. The numerical simulation framework, presented in this paper, is developed for the first time in order to incorporate an applied strain range that encompasses both

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the elastic and the post-peak constitutive behavior thereby achieving both strain and damage sensing by electrical measurements in these cementitious matrices. The modelling scheme involves: (1) generation of representative microstructure of the heterogeneous composite using a stochastic packing algorithm; (2) application of periodic boundary conditions [\[19–23\]](#page--1-5) in the representative unit cell to simulate a straincontrolled mechanical test scenario; (3) incorporation of interface damage to simulate interfacial debonding at the inclusion-matrix interface; (4) incorporation of an isotropic damage theory for damage in the matrix in the post-peak regime; (5) determination of effective constitutive behavior of the heterogeneous material; (6) re-meshing the deformed/damaged geometry corresponding to any specific applied strain and (7) determination of electrical response of the damaged/ deformed microstructure. Steps 6 and 7 are performed for strains both in the elastic and the post-peak regime to obtain change in electrical responses for all the applied strains. The versatility of this approach is verified on a smart self-sensing cementitious material enabled by nanoengineered matrix-inclusion interface $[24]$. This smart material uses thin multi walled carbon nanotube (MWCNT)-based polymeric films at the matrix-inclusion interface [\[15,16,24\]](#page--1-7). Thus, this paper intends to demonstrate a numerical framework to evaluate the strain- and damage-sensing efficiency of several heterogeneous materials facilitating microstructure-guided material design.

2. Numerical simulation framework for electro-mechanical response evaluation and damage detection

This section describes the framework which executes numerical simulation to evaluate electro-mechanical response of self-sensing materials using finite element analysis (FEA). Influence of damage and damage-sensing capability of the material is efficiently integrated into the simulation framework. [Fig. 1](#page-1-0) summarizes the numerical simulation framework using a flowchart representation.

The framework involves generation of a representative unit cell and evaluation of electromechanical responses implementing mechanical and electrical modules. The analysis framework is implemented here using a python script for ABAQUS™ solver. The mechanical module simulates a mechanical response of the unit cell under externally applied uniaxial strain and it accounts for interface damage at the matrixinclusion interface. In addition, the mechanical module implements constitutive behavior of heterogeneous composites beyond the cracking strain (post-peak response) by implementing an isotropic damage model [\[25–27\]](#page--1-8) in the matrix through a user-defined subroutine in ABAQUS[™] [\[28–30\].](#page--1-9) An intermediate remeshing module imports the deformed configuration of the unit cell, obtained from the mechanical module and improves the quality of mesh before exporting the re-meshed unit cell to the electrical module as a starting geometry for the electrical analysis in order to achieve electro-mechanical response of

Fig. 1. Flowchart of numerical simulation framework.

the unit cell under applied strain. The electrical module obtains the deformed configuration of the unit cell from the remeshing module and obtains current distribution in the deformed unit cell under imposed electrical potential. Post processing of the relevant electrical responses in MATLAB© yields a homogenized change in electrical resistivity under different applied strains. Different components of the framework are detailed in the forthcoming sub-sections.

2.1. Generation of representative unit cells

The unit cells are generated here using the Lubachhevsky-Stillinger algorithm [\[31–33\].](#page--1-10) This algorithm employs a hard contact model and hence particle overlaps are not allowed. First, the desired inclusions are randomly distributed inside the periodic bounding box with random initial velocities of the particles. The radius of each particle is first initialized as zero. The radius of ith particle (*ri*) in the next event is a function of the growth rate (g_i) , which is tailored to attain the desired particle size distribution shown in Eq. [\(1\)](#page-1-1).

$$
\frac{d\eta}{dt} = g_i \tag{1}
$$

Here $i = 1, 2, \ldots$ is the number of particles. The growth rate between time t^n and t^{n+1} is computed using a finite difference scheme as follows.

$$
g_i = \frac{(r_i^{n+1} - r_i^n)}{\Delta t} \tag{2}
$$

where r_i^{n+1} and r_i^n are radius at time t^n and t^{n+1} respectively and $\Delta t = (t^{n+1} - t^n)$. The particle radii are then updated as follows for time t^{n+1} by employing the growth rate and time increment (Δt) as follows.

$$
r_i^{n+1} = r_i^n + g_i \Delta t \tag{3}
$$

In addition, the position of particle '*i*' at time t^{n+1} i.e. \mathbf{x}_i^{n+1} is updated considering a constant velocity (v_i^n) between the time nodes.

$$
\mathbf{x}_{i}^{n+1} = \mathbf{x}_{i}^{n} + \mathbf{v}_{i}^{n} \Delta t
$$
 (4)

The vector that connects the centers of particles 'i' and 'j' is obtained by subtracting the position vectors of the two particles.

$$
\mathbf{I}_{ij}^{n+1} = \mathbf{x}_j^{n+1} - \mathbf{x}_i^{n+1} \tag{5}
$$

The particles 'i' and 'j' are expected to be in contact if the sum of their radii is equal to the length of the connection vector. The time step size can be calculated as follows and the formulations are adequately detailed in [\[34\].](#page--1-11)

$$
\Delta t = \min \left[\frac{-v \pm \sqrt{v^2 - uw}}{u} \right] \tag{6}
$$

where $\Delta t > 0$ and v, u and w are given as

$$
\mathbf{v} = \mathbf{I}_{ij}^n \cdot [\mathbf{v}_j^n - \mathbf{v}_i^n] - [r_i^n + r_j^n][g_i + g_j]
$$
\n
$$
(7a)
$$

$$
\mathbf{u} = [\mathbf{v}_j^n - \mathbf{v}_i^n]^2 - [g_i + g_j]^2 \tag{7b}
$$

$$
\mathbf{w} = \mathbf{I}_{ij}^{n^2} - [r_i^n + r_j^n]^2 \tag{7c}
$$

Here, \mathbf{v}_i^n and \mathbf{v}_j^n are the velocities of particles 'i' and 'j' at time t^n . r_i^n and r_j^n are the radius of particles 'i' and 'j' at time t^n . g_i and g_j are growth rates for particle 'i' and 'j' respectively. The vector connecting the position of the two particles at time t^n is given as $\mathbf{I}_{ij}^n = \mathbf{x}_j^n - \mathbf{x}_i^n$. The time step calculation (Eq. (6)) is performed for each particle pair that are being able to collide and thus minimum time step for all the possible collisions is adopted to move forward for the next event. All the particle positions x_i^{n+1} are updated using the forward Euler scheme (Eq. [\(4\)\)](#page-1-3) and new search for the next collision(s) is started. The post-contact velocities are computed as follows.

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